Getting integrated intensities out of powder diagrams

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With very highly resolved powder data, integrated intensities can be extracted which are sufficiently good to “solve” the structures of small proteins using single crystal molecular replacement software. These integrated intensities have some problems due to peak overlaps, but the molecular replacement softwares are tolerant, assuming the errors come from the structual model. These problems in our integrated intensities can be reduced both experimentally and also via more sophisticated software.

We have frequently been able to perturb the unit cells of protein microcrystals experimentally and so change the pattern of peak overlaps. By analysing several patterns at the same time we have been able to untangle some of the peaks which are overlapped in a single pattern. Some quality indicators for these combined datasets will be presented.

Unfortunately, in certain space group there are some inequivalent peaks which we will not be able to resolve in a powder diagram due to symmetry; for example the cubic (511) and (333) reflections. These are the same peaks which are overlapped in merohedrally twinned single crystals. With this in mind, we propose that the use of an “overlap” or “weight” matrix would be a useful way to unify the treatment of single crystal and powder data.